2-ethyl-3,5-dimethyl-tetrahydropyrazine

Inchi: InChI=1S/C8H16N2/c1-4-8-7(3)10-6(2)5-9-8/h6-7,10H,4-5H2,1-3H3
InchiKey: NBDKAZJVCZKVEC-UHFFFAOYSA-N
Formula: C8H16N2
SMILES: CCC1=NCC(C)NC1C
Mol. weight [g/mol]: 140.23

Physical Properties

Property code	Value	Unit	Source
gf	258.04	kJ/mol	Joback Method
hf	-19.38	kJ/mol	Joback Method
hfus	24.94	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.218		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1255.00		NIST Webbook
rinpol	1255.00		NIST Webbook
tb	503.71	K	Joback Method
tc	726.29	K	Joback Method
tf	372.91	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.26	J/mol×K	503.71	Joback Method
cpg	322.53	J/mol×K	540.81	Joback Method
cpg	339.98	J/mol×K	577.90	Joback Method
cpg	356.57	J/mol×K	615.00	Joback Method
cpg	372.31	J/mol×K	652.10	Joback Method
cpg	387.18	J/mol×K	689.20	Joback Method
cpg	401.15	J/mol×K	726.29	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume